Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2023 – 05:09 PM EDT

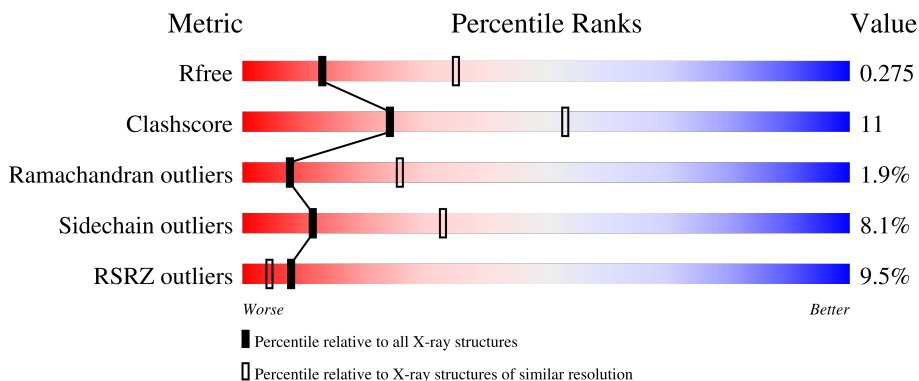|		
PDB ID	:	3VA6
Title	:	Crystal Structure of the extracellular domain of the putative hybrid two component system BT4673 from B. thetaiotaomicron
Authors	:	Zhang, Z.; Liu, Q.; Hendrickson, W.A.
Deposited on	:	2011-12-28
Resolution	:	2.80 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
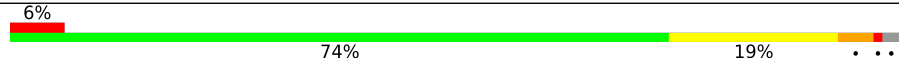*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.275
Clashscore		11
Ramachandran outliers		1.9%
Sidechain outliers		8.1%
RSRZ outliers		9.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	758	13% · · · 77% · · 18% · ·
1	B	758	6% · · · 74% · · 19% · · ·

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 12203 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Two-component system sensor histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total 6077	C 3855	N 1043	O 1162	S 17	0	0	0
1	B	743	Total 6032	C 3828	N 1028	O 1158	S 18	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	LEU	-	expression tag	UNP Q89YQ8
A	29	GLU	-	expression tag	UNP Q89YQ8
A	778	LEU	-	expression tag	UNP Q89YQ8
A	779	GLU	-	expression tag	UNP Q89YQ8
A	780	HIS	-	expression tag	UNP Q89YQ8
A	781	HIS	-	expression tag	UNP Q89YQ8
A	782	HIS	-	expression tag	UNP Q89YQ8
A	783	HIS	-	expression tag	UNP Q89YQ8
A	784	HIS	-	expression tag	UNP Q89YQ8
A	785	HIS	-	expression tag	UNP Q89YQ8
B	28	LEU	-	expression tag	UNP Q89YQ8
B	29	GLU	-	expression tag	UNP Q89YQ8
B	778	LEU	-	expression tag	UNP Q89YQ8
B	779	GLU	-	expression tag	UNP Q89YQ8
B	780	HIS	-	expression tag	UNP Q89YQ8
B	781	HIS	-	expression tag	UNP Q89YQ8
B	782	HIS	-	expression tag	UNP Q89YQ8
B	783	HIS	-	expression tag	UNP Q89YQ8
B	784	HIS	-	expression tag	UNP Q89YQ8
B	785	HIS	-	expression tag	UNP Q89YQ8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	48	Total O 48 48		0	0
2	B	46	Total O 46 46		0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Two-component system sensor histidine kinase

Chain A:

• Molecule 1: Two-component system sensor histidine kinase

Chain B:
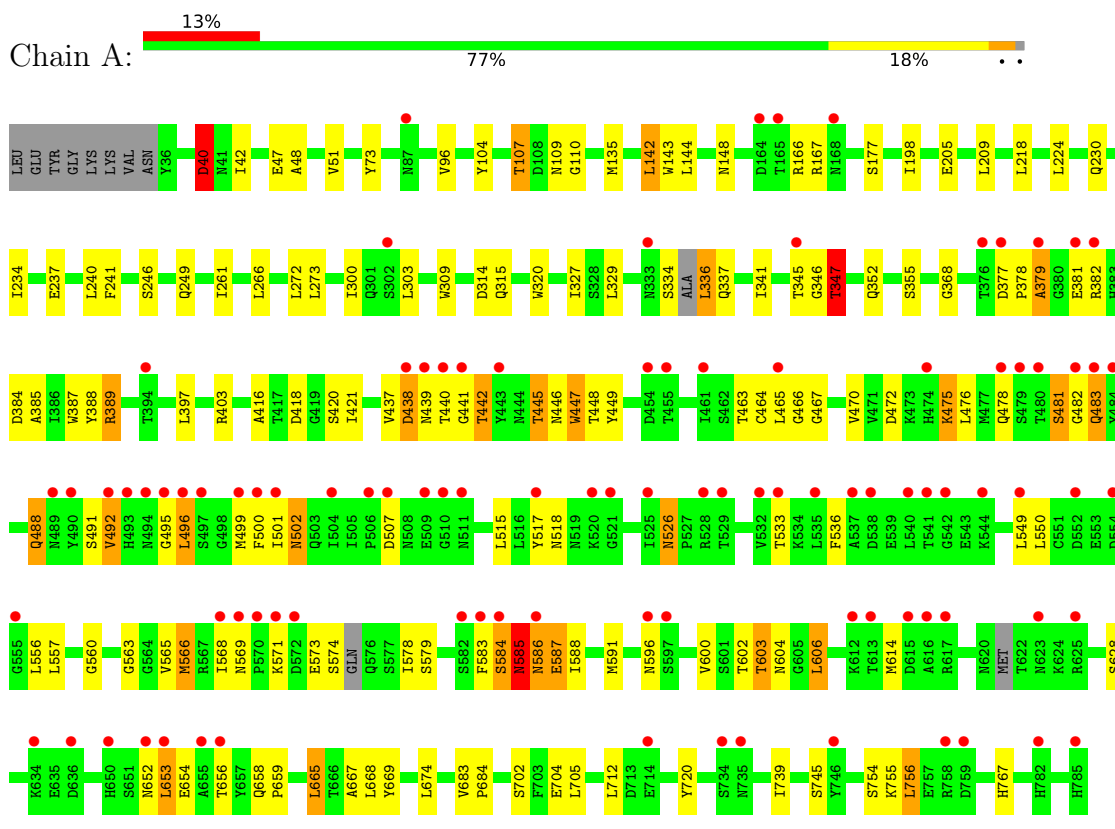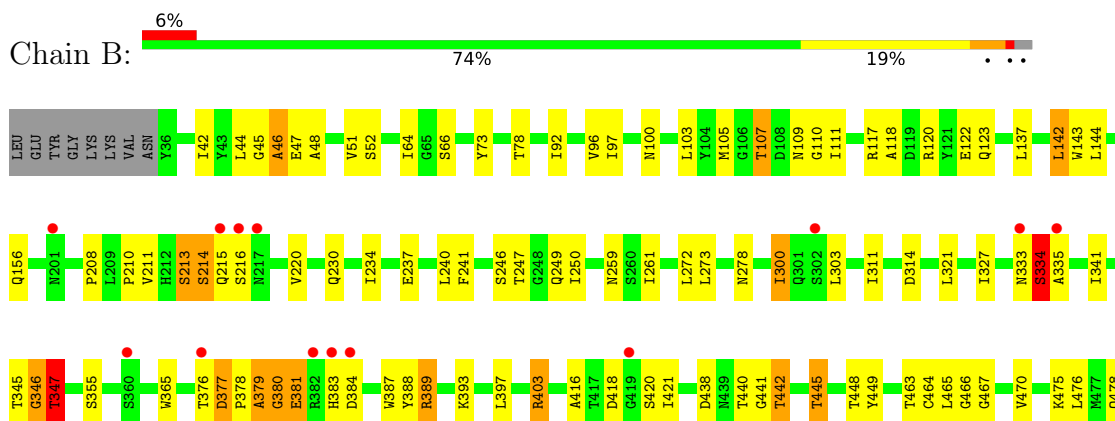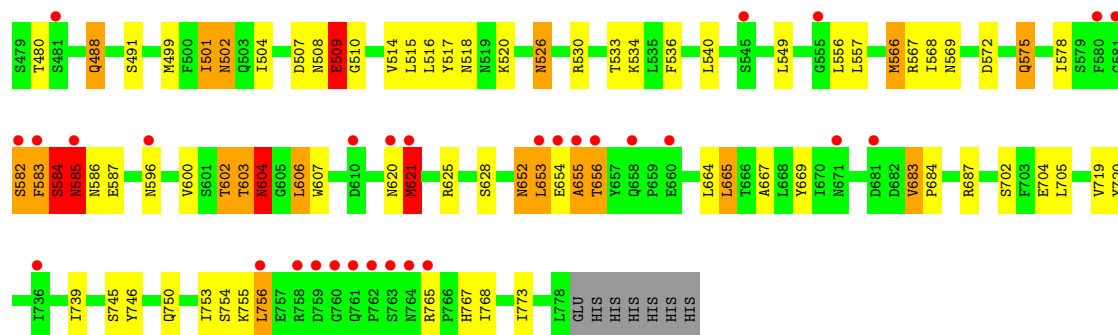
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	87.88Å 87.88Å 430.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.86 – 2.80 45.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.2 (45.86-2.80) 92.3 (45.86-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.91 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.216 , 0.274 0.218 , 0.275	Depositor DCC
R_{free} test set	2024 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	1.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.3	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12203	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.65	4/6232 (0.1%)	0.74	1/8466 (0.0%)
1	B	0.68	2/6184 (0.0%)	0.79	4/8405 (0.0%)
All	All	0.67	6/12416 (0.0%)	0.76	5/16871 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	TRP	CD2-CE2	5.53	1.48	1.41
1	B	365	TRP	CD2-CE2	5.26	1.47	1.41
1	A	143	TRP	CD2-CE2	5.15	1.47	1.41
1	A	320	TRP	CD2-CE2	5.06	1.47	1.41
1	B	607	TRP	CD2-CE2	5.04	1.47	1.41
1	A	447	TRP	CD2-CE2	5.04	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
1	B	403	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	380	GLY	N-CA-C	5.32	126.39	113.10
1	B	509	GLU	N-CA-C	-5.20	96.96	111.00
1	B	530	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	40	ASP	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	213	SER	Peptide
1	B	441	GLY	Peptide
1	B	508	ASN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6077	0	5785	119	0
1	B	6032	0	5767	146	0
2	A	48	0	0	1	0
2	B	46	0	0	4	0
All	All	12203	0	11552	260	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (260) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ASN:HB3	1:A:587:GLU:HA	1.26	1.06
1:A:166:ARG:HG3	1:A:166:ARG:HH11	1.28	0.97
1:B:46:ALA:H	1:B:47:GLU:HA	1.32	0.92
1:A:578:ILE:HG23	1:A:614:MET:CE	2.00	0.90
1:A:586:ASN:HB3	1:A:587:GLU:CA	2.02	0.89
1:A:586:ASN:CB	1:A:587:GLU:HA	2.02	0.89
1:B:420:SER:OG	1:B:445:THR:HG22	1.74	0.88
1:A:585:ASN:O	1:A:586:ASN:HB2	1.74	0.88
1:A:578:ILE:HG23	1:A:614:MET:HE2	1.54	0.87
1:B:584:SER:OG	1:B:585:ASN:HB3	1.75	0.86
1:B:584:SER:CB	1:B:585:ASN:HB3	2.06	0.86
1:A:658:GLN:NE2	1:A:712:LEU:HD21	1.92	0.83
1:A:345:THR:HG23	1:A:385:ALA:HB3	1.62	0.81
1:A:420:SER:OG	1:A:445:THR:HG22	1.80	0.80
1:A:96:VAL:HG12	1:A:135:MET:CE	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:GLY:O	1:B:46:ALA:HB2	1.82	0.79
1:B:517:TYR:CE2	1:B:518:ASN:ND2	2.52	0.78
1:B:120:ARG:NE	1:B:122:GLU:OE2	2.17	0.77
1:B:463:THR:HG22	1:B:466:GLY:H	1.50	0.77
1:A:230:GLN:HE21	1:B:230:GLN:NE2	1.82	0.77
1:A:584:SER:N	1:A:585:ASN:O	2.18	0.76
1:B:45:GLY:O	1:B:46:ALA:CB	2.34	0.76
1:B:569:ASN:O	1:B:572:ASP:O	2.04	0.75
1:B:475:LYS:HE2	2:B:820:HOH:O	1.85	0.75
1:B:333:ASN:O	1:B:334:SER:HB2	1.87	0.74
1:A:230:GLN:HE21	1:B:230:GLN:HE21	1.32	0.73
1:A:378:PRO:O	1:A:379:ALA:HB2	1.87	0.73
1:B:380:GLY:O	1:B:381:GLU:HB2	1.88	0.73
1:B:750:GLN:HE21	1:B:768:ILE:HG21	1.54	0.72
1:A:584:SER:HA	1:A:585:ASN:O	1.89	0.72
1:B:667:ALA:HB3	1:B:704:GLU:HB2	1.71	0.72
1:A:492:VAL:HG11	1:A:499:MET:CE	2.19	0.72
1:A:96:VAL:HG12	1:A:135:MET:HE3	1.71	0.71
1:B:247:THR:OG1	1:B:249:GLN:HG3	1.90	0.71
1:B:750:GLN:HE21	1:B:768:ILE:CG2	2.05	0.70
1:B:583:PHE:O	1:B:586:ASN:ND2	2.25	0.70
1:A:346:GLY:HA2	1:A:347:THR:O	1.93	0.69
1:A:658:GLN:HE21	1:A:712:LEU:HD21	1.57	0.69
1:A:584:SER:CA	1:A:585:ASN:O	2.41	0.69
1:A:403:ARG:NH2	1:B:156:GLN:O	2.26	0.69
1:B:377:ASP:O	1:B:383:HIS:ND1	2.26	0.69
1:A:40:ASP:OD2	1:A:329:LEU:HD23	1.93	0.68
1:B:142:LEU:HD13	1:B:144:LEU:HD21	1.74	0.68
1:B:118:ALA:HB1	1:B:120:ARG:HD3	1.75	0.68
1:A:563:GLY:HA2	1:A:586:ASN:ND2	2.08	0.68
1:B:526:ASN:C	1:B:526:ASN:HD22	1.98	0.67
1:A:166:ARG:HG3	1:A:166:ARG:NH1	2.07	0.67
1:B:208:PRO:O	1:B:250:ILE:HD13	1.94	0.67
1:A:378:PRO:O	1:A:379:ALA:CB	2.40	0.66
1:B:440:THR:OG1	1:B:442:THR:HG23	1.95	0.66
1:B:416:ALA:HB1	1:B:448:THR:HG22	1.77	0.66
1:B:520:LYS:HE3	2:B:816:HOH:O	1.94	0.66
1:A:585:ASN:O	1:A:586:ASN:CB	2.44	0.66
1:A:416:ALA:HB1	1:A:448:THR:HG22	1.77	0.65
1:B:379:ALA:C	1:B:383:HIS:HE1	2.00	0.65
1:A:96:VAL:CG1	1:A:135:MET:HE3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:GLY:HA2	1:B:347:THR:O	1.98	0.64
1:B:215:GLN:CD	1:B:216:SER:HA	2.18	0.64
1:A:475:LYS:HD3	1:A:475:LYS:N	2.13	0.64
1:B:421:ILE:CG2	1:B:448:THR:HG21	2.28	0.64
1:A:166:ARG:HH11	1:A:166:ARG:CG	2.06	0.64
1:B:214:SER:OG	1:B:215:GLN:HG2	1.98	0.64
1:B:215:GLN:CB	1:B:216:SER:HA	2.27	0.64
1:A:96:VAL:HG12	1:A:135:MET:HE1	1.79	0.63
1:B:584:SER:CA	1:B:585:ASN:HB3	2.27	0.63
1:B:566:MET:HE2	1:B:568:ILE:HD11	1.79	0.63
1:A:421:ILE:CG2	1:A:448:THR:HG21	2.29	0.63
1:A:463:THR:HG22	1:A:466:GLY:H	1.62	0.63
1:B:143:TRP:O	1:B:144:LEU:HD23	2.00	0.62
1:B:582:SER:O	1:B:583:PHE:HB2	2.00	0.61
1:A:502:ASN:HB3	1:A:515:LEU:HD12	1.80	0.61
1:A:602:THR:HG22	1:A:604:ASN:N	2.15	0.61
1:B:536:PHE:HB3	1:B:566:MET:HE1	1.81	0.61
1:A:526:ASN:HD22	1:A:526:ASN:C	2.02	0.61
1:B:566:MET:SD	1:B:575:GLN:HG3	2.40	0.60
1:A:445:THR:O	1:A:445:THR:CG2	2.50	0.60
1:B:501:ILE:HG22	1:B:516:LEU:HG	1.83	0.59
1:A:602:THR:HG22	1:A:604:ASN:H	1.66	0.59
1:A:492:VAL:HG11	1:A:499:MET:HE1	1.83	0.59
1:B:655:ALA:HA	1:B:656:THR:C	2.21	0.59
1:B:421:ILE:HG22	1:B:448:THR:HG21	1.85	0.58
1:B:502:ASN:HB2	1:B:515:LEU:HD12	1.84	0.58
1:A:104:TYR:O	1:A:135:MET:HE1	2.02	0.58
1:B:215:GLN:NE2	1:B:216:SER:HA	2.19	0.58
1:B:378:PRO:O	1:B:379:ALA:HB2	2.04	0.58
1:B:475:LYS:CE	2:B:820:HOH:O	2.46	0.57
1:B:46:ALA:N	1:B:47:GLU:HA	2.06	0.57
1:A:437:VAL:HG23	1:A:438:ASP:O	2.04	0.57
1:A:464:CYS:O	1:A:465:LEU:HB2	2.04	0.57
1:B:311:ILE:HG23	1:B:321:LEU:HD23	1.86	0.57
1:B:334:SER:CB	1:B:335:ALA:HA	2.35	0.57
1:A:665:LEU:HD22	1:A:767:HIS:NE2	2.19	0.56
1:A:142:LEU:HD13	1:A:144:LEU:HD21	1.87	0.56
1:B:51:VAL:HG13	1:B:64:ILE:HG23	1.86	0.56
1:B:272:LEU:HD13	1:B:273:LEU:N	2.20	0.56
1:B:540:LEU:HD11	1:B:566:MET:HE2	1.88	0.56
1:B:566:MET:CE	1:B:568:ILE:HD11	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:THR:HG22	1:B:604:ASN:CB	2.36	0.56
1:A:345:THR:HG23	1:A:385:ALA:CB	2.34	0.56
1:B:463:THR:HB	1:B:467:GLY:O	2.06	0.56
1:A:345:THR:CG2	1:A:385:ALA:HB3	2.35	0.56
1:A:587:GLU:N	1:A:603:THR:OG1	2.38	0.56
1:B:107:THR:HG22	1:B:109:ASN:N	2.21	0.55
1:A:42:ILE:HD13	1:A:73:TYR:CE2	2.41	0.55
1:A:237:GLU:HG3	2:A:838:HOH:O	2.06	0.55
1:B:578:ILE:C	1:B:578:ILE:HD12	2.27	0.55
1:B:420:SER:OG	1:B:445:THR:CG2	2.51	0.55
1:A:674:LEU:HD23	1:A:674:LEU:C	2.26	0.55
1:B:602:THR:HG22	1:B:604:ASN:HB2	1.88	0.55
1:A:492:VAL:HG11	1:A:499:MET:HE2	1.87	0.54
1:B:475:LYS:O	1:B:476:LEU:HB3	2.07	0.54
1:A:51:VAL:HG21	1:A:327:ILE:HG13	1.90	0.54
1:A:463:THR:HB	1:A:467:GLY:O	2.07	0.54
1:B:272:LEU:HD13	1:B:272:LEU:C	2.28	0.54
1:A:421:ILE:HG22	1:A:448:THR:HG21	1.90	0.54
1:B:381:GLU:H	1:B:383:HIS:CE1	2.25	0.54
1:B:584:SER:CB	1:B:585:ASN:CB	2.82	0.54
1:B:664:LEU:HD23	1:B:687:ARG:HG3	1.90	0.54
1:B:379:ALA:C	1:B:383:HIS:CE1	2.80	0.53
1:B:509:GLU:HG3	1:B:510:GLY:H	1.72	0.53
1:A:683:VAL:HG12	1:A:684:PRO:HD2	1.90	0.53
1:A:475:LYS:N	1:A:475:LYS:CD	2.72	0.53
1:B:504:ILE:HG22	1:B:514:VAL:HG13	1.90	0.53
1:A:166:ARG:NH1	1:A:166:ARG:CG	2.69	0.53
1:A:583:PHE:HA	1:A:584:SER:C	2.29	0.52
1:A:107:THR:HG22	1:A:109:ASN:N	2.25	0.52
1:A:517:TYR:CE2	1:A:518:ASN:ND2	2.77	0.52
1:B:602:THR:CG2	1:B:604:ASN:HB2	2.40	0.52
1:A:272:LEU:C	1:A:272:LEU:HD13	2.29	0.52
1:B:445:THR:CG2	1:B:445:THR:O	2.58	0.52
1:B:750:GLN:NE2	1:B:768:ILE:HG21	2.23	0.52
1:A:492:VAL:N	1:A:495:GLY:O	2.44	0.51
1:B:509:GLU:CG	1:B:510:GLY:H	2.23	0.51
1:B:583:PHE:HA	1:B:584:SER:CB	2.41	0.51
1:B:381:GLU:HA	1:B:383:HIS:CD2	2.46	0.51
1:B:683:VAL:HG12	1:B:684:PRO:HD2	1.92	0.51
1:B:665:LEU:HD22	1:B:767:HIS:NE2	2.26	0.51
1:A:381:GLU:HB3	1:B:393:LYS:NZ	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:TYR:CE1	1:B:464:CYS:HB2	2.47	0.50
1:B:584:SER:OG	1:B:585:ASN:CB	2.53	0.50
1:B:107:THR:CG2	1:B:109:ASN:H	2.25	0.50
1:B:118:ALA:CB	1:B:120:ARG:HD3	2.41	0.49
1:B:470:VAL:HB	1:B:488:GLN:HG3	1.94	0.49
1:A:658:GLN:NE2	1:A:712:LEU:CD2	2.70	0.49
1:B:142:LEU:HD22	1:B:143:TRP:O	2.13	0.49
1:B:719:VAL:HG13	1:B:756:LEU:HD13	1.95	0.49
1:B:705:LEU:HD22	1:B:753:ILE:HD13	1.94	0.49
1:B:379:ALA:O	1:B:383:HIS:CE1	2.65	0.49
1:A:224:LEU:HD21	1:A:266:LEU:HG	1.93	0.49
1:A:107:THR:HG22	1:A:110:GLY:H	1.78	0.49
1:A:667:ALA:HB3	1:A:704:GLU:HB2	1.93	0.49
1:B:572:ASP:O	1:B:572:ASP:OD1	2.31	0.48
1:A:560:GLY:HA2	1:A:565:VAL:HG12	1.95	0.48
1:B:765:ARG:NH1	2:B:830:HOH:O	2.45	0.48
1:A:107:THR:HG22	1:A:110:GLY:N	2.28	0.48
1:B:540:LEU:HD11	1:B:566:MET:CE	2.43	0.48
1:A:720:TYR:CE2	1:A:739:ILE:HG23	2.48	0.48
1:A:652:ASN:C	1:A:654:GLU:H	2.16	0.48
1:A:439:ASN:OD1	1:A:440:THR:HG23	2.14	0.48
1:A:47:GLU:HG3	1:A:48:ALA:N	2.29	0.47
1:B:208:PRO:O	1:B:250:ILE:CD1	2.62	0.47
1:B:654:GLU:O	1:B:655:ALA:C	2.52	0.47
1:A:556:LEU:HD23	1:A:569:ASN:HA	1.94	0.47
1:A:578:ILE:HG23	1:A:614:MET:HE3	1.91	0.47
1:A:600:VAL:O	1:A:606:LEU:HD23	2.15	0.47
1:A:578:ILE:CG2	1:A:614:MET:HE2	2.36	0.47
1:B:620:ASN:O	1:B:621:MET:C	2.53	0.47
1:B:107:THR:HG22	1:B:110:GLY:N	2.29	0.47
1:B:345:THR:OG1	1:B:346:GLY:N	2.47	0.47
1:A:569:ASN:HB3	1:A:573:GLU:CB	2.45	0.47
1:B:240:LEU:HB2	1:B:261:ILE:CD1	2.45	0.47
1:A:563:GLY:HA2	1:A:586:ASN:HD22	1.78	0.47
1:B:516:LEU:HD12	1:B:516:LEU:N	2.30	0.46
1:B:584:SER:N	1:B:585:ASN:HB3	2.29	0.46
1:A:470:VAL:HB	1:A:488:GLN:HG3	1.97	0.46
1:B:42:ILE:HD13	1:B:73:TYR:CE2	2.50	0.46
1:B:48:ALA:HB1	1:B:66:SER:HB2	1.97	0.46
1:B:97:ILE:HG12	1:B:103:LEU:CD2	2.44	0.46
1:B:381:GLU:N	1:B:383:HIS:CE1	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:720:TYR:CE2	1:B:739:ILE:HG23	2.51	0.46
1:A:387:TRP:CD1	1:A:389:ARG:HD2	2.50	0.46
1:A:107:THR:CG2	1:A:109:ASN:H	2.29	0.46
1:B:475:LYS:O	1:B:476:LEU:CB	2.61	0.46
1:A:495:GLY:O	1:A:496:LEU:HB2	2.15	0.46
1:A:566:MET:HG2	1:A:568:ILE:HD11	1.97	0.46
1:B:44:LEU:HD23	1:B:78:THR:HG21	1.97	0.46
1:B:445:THR:O	1:B:445:THR:HG23	2.15	0.46
1:A:272:LEU:HD13	1:A:273:LEU:N	2.31	0.46
1:A:669:TYR:HB2	1:A:702:SER:HB2	1.98	0.46
1:B:259:ASN:HD21	1:B:278:ASN:HB2	1.81	0.46
1:B:491:SER:HB2	1:B:499:MET:SD	2.56	0.46
1:A:569:ASN:HB3	1:A:573:GLU:HB3	1.96	0.46
1:B:220:VAL:HG13	1:B:234:ILE:HG23	1.98	0.46
1:B:463:THR:CG2	1:B:466:GLY:H	2.23	0.45
1:A:334:SER:HG	1:A:336:LEU:N	2.14	0.45
1:A:441:GLY:HA2	1:A:442:THR:O	2.15	0.45
1:A:445:THR:O	1:A:445:THR:HG23	2.15	0.45
1:A:578:ILE:C	1:A:578:ILE:HD12	2.36	0.45
1:B:51:VAL:HG21	1:B:327:ILE:HG13	1.98	0.45
1:A:381:GLU:HB3	1:B:393:LYS:HZ1	1.82	0.45
1:B:92:ILE:HG23	1:B:105:MET:HB3	1.99	0.45
1:A:550:LEU:HD12	1:A:550:LEU:C	2.37	0.45
1:A:209:LEU:HD21	1:A:234:ILE:HD13	1.98	0.44
1:B:300:ILE:HG23	1:B:300:ILE:O	2.15	0.44
1:B:52:SER:OG	1:B:92:ILE:O	2.30	0.44
1:B:387:TRP:CD1	1:B:389:ARG:HD2	2.53	0.44
1:A:240:LEU:HB2	1:A:261:ILE:CD1	2.47	0.44
1:A:756:LEU:HD12	1:A:756:LEU:HA	1.91	0.44
1:A:482:GLY:N	1:A:483:GLN:O	2.47	0.44
1:B:46:ALA:H	1:B:47:GLU:CA	2.18	0.44
1:B:388:TYR:HB3	1:B:397:LEU:HG	2.00	0.44
1:A:482:GLY:HA3	1:A:483:GLN:CB	2.47	0.44
1:A:536:PHE:HE1	1:A:574:SER:HB3	1.83	0.44
1:B:240:LEU:HB2	1:B:261:ILE:HD12	1.99	0.44
1:B:652:ASN:CG	1:B:653:LEU:H	2.20	0.44
1:B:311:ILE:HG23	1:B:321:LEU:CD2	2.47	0.43
1:B:314:ASP:OD2	1:B:314:ASP:C	2.57	0.43
1:B:665:LEU:HD22	1:B:767:HIS:CD2	2.54	0.43
1:A:314:ASP:OD2	1:A:314:ASP:C	2.57	0.43
1:B:600:VAL:O	1:B:606:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:THR:HG22	1:B:110:GLY:H	1.82	0.43
1:B:669:TYR:HB2	1:B:702:SER:HB2	1.99	0.43
1:A:591:MET:HG2	1:A:600:VAL:HG13	2.00	0.43
1:B:719:VAL:HG13	1:B:756:LEU:CD1	2.49	0.43
1:B:234:ILE:HB	1:B:241:PHE:HB2	2.01	0.43
1:B:509:GLU:HG3	1:B:510:GLY:N	2.33	0.43
1:B:567:ARG:O	1:B:575:GLN:HA	2.19	0.42
1:A:300:ILE:O	1:A:300:ILE:HG23	2.18	0.42
1:B:526:ASN:C	1:B:526:ASN:ND2	2.67	0.42
1:B:47:GLU:HA	1:B:47:GLU:OE1	2.19	0.42
1:B:746:TYR:HA	1:B:773:ILE:HB	2.01	0.42
1:A:665:LEU:HD22	1:A:767:HIS:CD2	2.54	0.42
1:B:585:ASN:CG	1:B:586:ASN:N	2.73	0.42
1:B:215:GLN:HB3	1:B:216:SER:HA	2.00	0.41
1:B:100:ASN:O	1:B:117:ARG:NH1	2.50	0.41
1:B:272:LEU:C	1:B:272:LEU:CD1	2.89	0.41
1:B:335:ALA:O	1:B:655:ALA:HB1	2.21	0.41
1:B:378:PRO:O	1:B:379:ALA:CB	2.67	0.41
1:A:652:ASN:O	1:A:654:GLU:N	2.47	0.41
1:B:377:ASP:O	1:B:383:HIS:CE1	2.73	0.41
1:B:111:ILE:O	1:B:123:GLN:NE2	2.54	0.41
1:B:111:ILE:HD11	1:B:144:LEU:HD13	2.02	0.41
1:B:210:PRO:CD	1:B:250:ILE:HG21	2.51	0.41
1:B:403:ARG:NH1	1:B:418:ASP:OD2	2.54	0.41
1:A:198:ILE:HD11	1:A:205:GLU:HB2	2.03	0.41
1:A:337:GLN:OE1	1:A:659:PRO:HB3	2.20	0.41
1:B:333:ASN:O	1:B:334:SER:CB	2.64	0.41
1:A:403:ARG:NH1	1:A:418:ASP:OD2	2.54	0.41
1:A:449:TYR:CE1	1:A:464:CYS:HB2	2.56	0.41
1:B:107:THR:CG2	1:B:109:ASN:N	2.84	0.41
1:A:234:ILE:HB	1:A:241:PHE:HB2	2.03	0.40
1:A:560:GLY:CA	1:A:588:ILE:HD12	2.51	0.40
1:A:388:TYR:HB3	1:A:397:LEU:HG	2.03	0.40
1:A:446:ASN:HD22	1:A:446:ASN:HA	1.73	0.40
1:A:447:TRP:CZ3	1:A:465:LEU:HD12	2.56	0.40
1:A:586:ASN:C	1:A:603:THR:OG1	2.59	0.40
1:A:668:LEU:HD23	1:A:683:VAL:HG11	2.03	0.40
1:A:705:LEU:C	1:A:705:LEU:HD12	2.41	0.40
1:A:352:GLN:O	1:A:368:GLY:HA3	2.22	0.40
1:A:107:THR:CG2	1:A:109:ASN:N	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/758 (98%)	682 (92%)	46 (6%)	11 (2%)	10	33
1	B	741/758 (98%)	685 (92%)	39 (5%)	17 (2%)	6	21
All	All	1480/1516 (98%)	1367 (92%)	85 (6%)	28 (2%)	8	26

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ALA
1	A	492	VAL
1	A	585	ASN
1	A	586	ASN
1	B	46	ALA
1	B	334	SER
1	B	379	ALA
1	B	582	SER
1	B	583	PHE
1	B	585	ASN
1	B	604	ASN
1	A	347	THR
1	A	442	THR
1	A	496	LEU
1	B	346	GLY
1	B	347	THR
1	B	381	GLU
1	B	603	THR
1	B	621	MET
1	B	655	ALA
1	A	481	SER
1	A	502	ASN
1	A	653	LEU
1	B	502	ASN
1	B	652	ASN

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Mol	Chain	Res	Type
1	B	214	SER
1	B	584	SER
1	A	483	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	666/676 (98%)	614 (92%)	52 (8%)	12	35
1	B	662/676 (98%)	607 (92%)	55 (8%)	11	32
All	All	1328/1352 (98%)	1221 (92%)	107 (8%)	11	33

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	107	THR
1	A	142	LEU
1	A	148	ASN
1	A	167	ARG
1	A	177	SER
1	A	218	LEU
1	A	246	SER
1	A	249	GLN
1	A	303	LEU
1	A	315	GLN
1	A	336	LEU
1	A	341	ILE
1	A	347	THR
1	A	355	SER
1	A	377	ASP
1	A	382	ARG
1	A	384	ASP
1	A	389	ARG
1	A	438	ASP

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Mol	Chain	Res	Type
1	A	445	THR
1	A	472	ASP
1	A	475	LYS
1	A	476	LEU
1	A	478	GLN
1	A	481	SER
1	A	488	GLN
1	A	491	SER
1	A	500	PHE
1	A	501	ILE
1	A	507	ASP
1	A	526	ASN
1	A	533	THR
1	A	549	LEU
1	A	557	LEU
1	A	566	MET
1	A	571	LYS
1	A	579	SER
1	A	584	SER
1	A	585	ASN
1	A	587	GLU
1	A	596	ASN
1	A	603	THR
1	A	606	LEU
1	A	628	SER
1	A	653	LEU
1	A	656	THR
1	A	665	LEU
1	A	745	SER
1	A	754	SER
1	A	755	LYS
1	A	756	LEU
1	B	96	VAL
1	B	107	THR
1	B	137	LEU
1	B	142	LEU
1	B	211	VAL
1	B	213	SER
1	B	237	GLU
1	B	246	SER
1	B	300	ILE
1	B	303	LEU

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Mol	Chain	Res	Type
1	B	334	SER
1	B	341	ILE
1	B	347	THR
1	B	355	SER
1	B	376	THR
1	B	377	ASP
1	B	384	ASP
1	B	389	ARG
1	B	438	ASP
1	B	442	THR
1	B	445	THR
1	B	465	LEU
1	B	478	GLN
1	B	480	THR
1	B	488	GLN
1	B	501	ILE
1	B	507	ASP
1	B	509	GLU
1	B	526	ASN
1	B	533	THR
1	B	534	LYS
1	B	549	LEU
1	B	556	LEU
1	B	557	LEU
1	B	566	MET
1	B	575	GLN
1	B	584	SER
1	B	585	ASN
1	B	587	GLU
1	B	596	ASN
1	B	602	THR
1	B	603	THR
1	B	604	ASN
1	B	606	LEU
1	B	621	MET
1	B	625	ARG
1	B	628	SER
1	B	653	LEU
1	B	656	THR
1	B	665	LEU
1	B	683	VAL
1	B	745	SER

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Mol	Chain	Res	Type
1	B	754	SER
1	B	755	LYS
1	B	756	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
1	A	249	GLN
1	A	343	GLN
1	A	446	ASN
1	A	511	ASN
1	A	518	ASN
1	A	526	ASN
1	A	586	ASN
1	A	658	GLN
1	A	673	GLN
1	A	750	GLN
1	A	783	HIS
1	A	784	HIS
1	B	215	GLN
1	B	230	GLN
1	B	242	GLN
1	B	333	ASN
1	B	383	HIS
1	B	446	ASN
1	B	483	GLN
1	B	502	ASN
1	B	518	ASN
1	B	526	ASN
1	B	586	ASN
1	B	750	GLN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

5.4　Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	747/758 (98%)	0.87	98 (13%)	3	2	55, 70, 123, 152	6 (0%)
1	B	743/758 (98%)	0.58	43 (5%)	23	15	54, 65, 88, 112	7 (0%)
All	All	1490/1516 (98%)	0.73	141 (9%)	8	4	54, 67, 112, 152	13 (0%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	ASN	5.9
1	B	384	ASP	5.8
1	B	655	ALA	5.8
1	A	583	PHE	5.5
1	A	440	THR	5.4
1	A	478	GLN	4.6
1	A	656	THR	4.6
1	A	538	ASP	4.6
1	B	582	SER	4.6
1	A	482	GLY	4.5
1	A	499	MET	4.5
1	B	764	ASN	4.4
1	A	443	TYR	4.2
1	B	333	ASN	4.1
1	A	438	ASP	4.0
1	A	506	PRO	4.0
1	A	540	LEU	4.0
1	A	597	SER	4.0
1	A	572	ASP	4.0
1	B	653	LEU	3.8
1	B	760	GLY	3.7
1	B	583	PHE	3.7
1	B	656	THR	3.6
1	A	615	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	636	ASP	3.6
1	A	584	SER	3.5
1	B	581	GLY	3.5
1	A	455	THR	3.4
1	B	654	GLU	3.4
1	B	382	ARG	3.4
1	A	554	ASP	3.4
1	A	379	ALA	3.3
1	A	746	TYR	3.3
1	A	586	ASN	3.3
1	B	758	ARG	3.2
1	A	480	THR	3.2
1	A	653	LEU	3.1
1	B	765	ARG	3.1
1	A	616	ALA	3.1
1	A	617	ARG	3.1
1	A	381	GLU	3.0
1	B	215	GLN	3.0
1	A	759	ASP	3.0
1	B	761	GLN	3.0
1	A	582	SER	3.0
1	A	489	ASN	2.9
1	A	571	LYS	2.9
1	B	759	ASP	2.9
1	A	454	ASP	2.9
1	A	613	THR	2.9
1	A	165	THR	2.8
1	A	532	VAL	2.8
1	A	782	HIS	2.8
1	B	217	ASN	2.8
1	A	714	GLU	2.8
1	A	394	THR	2.7
1	A	345	THR	2.7
1	A	537	ALA	2.7
1	A	509	GLU	2.7
1	A	497	SER	2.7
1	B	335	ALA	2.6
1	A	493	HIS	2.6
1	A	544	LYS	2.6
1	A	496	LEU	2.6
1	A	168	ASN	2.6
1	A	507	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	623	ASN	2.6
1	A	441	GLY	2.6
1	B	216	SER	2.6
1	B	596	ASN	2.5
1	A	333	ASN	2.5
1	A	377	ASP	2.5
1	A	490	TYR	2.5
1	B	360	SER	2.4
1	A	596	ASN	2.4
1	A	500	PHE	2.4
1	A	655	ALA	2.4
1	A	549	LEU	2.4
1	A	533	THR	2.4
1	A	735	ASN	2.4
1	B	555	GLY	2.4
1	A	382	ARG	2.4
1	A	555	GLY	2.4
1	A	652	ASN	2.4
1	A	535	LEU	2.4
1	A	521	GLY	2.4
1	A	517	TYR	2.4
1	A	479	SER	2.3
1	B	481	SER	2.3
1	A	474	HIS	2.3
1	A	495	GLY	2.3
1	A	542	GLY	2.3
1	A	634	LYS	2.3
1	A	528	ARG	2.3
1	A	484	TYR	2.3
1	A	492	VAL	2.3
1	A	511	ASN	2.3
1	B	620	ASN	2.3
1	A	376	THR	2.2
1	A	785	HIS	2.2
1	B	671	ASN	2.2
1	A	504	ILE	2.2
1	A	510	GLY	2.2
1	B	660	GLU	2.2
1	A	541	THR	2.2
1	A	569	ASN	2.2
1	B	610	ASP	2.2
1	A	570	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	164	ASP	2.2
1	B	383	HIS	2.2
1	A	520	LYS	2.2
1	A	525	ILE	2.2
1	B	545	SER	2.2
1	B	762	PRO	2.2
1	A	87	ASN	2.1
1	B	763	SER	2.1
1	B	681	ASP	2.1
1	B	376	THR	2.1
1	A	465	LEU	2.1
1	A	552	ASP	2.1
1	A	625	ARG	2.1
1	B	585	ASN	2.1
1	B	621	MET	2.1
1	A	302	SER	2.1
1	B	419	GLY	2.1
1	A	501	ILE	2.1
1	B	201	ASN	2.1
1	A	650	HIS	2.1
1	A	734	SER	2.1
1	B	580	PHE	2.1
1	A	568	ILE	2.1
1	A	529	THR	2.1
1	B	736	ILE	2.1
1	A	758	ARG	2.0
1	A	612	LYS	2.0
1	A	461	ILE	2.0
1	A	439	ASN	2.0
1	A	483	GLN	2.0
1	B	658	GLN	2.0
1	B	302	SER	2.0
1	B	756	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.